Final Technical Report

N00014-88-K-0099

Microscopic Studies of Clusters in Phase Transitions

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During the period 1 October 1987 to 30 September 1990 research was done on the following projects.

1. Structure of Clusters in meanfield percolation models.

The fractal properties of percolation clusters in the long range bond or meanfield limit were investigated via Monte Carlo simulations and by the use of scaling arguments. These investigations were undertaken because it is these meanfield structures that initiate nucleation near the spinodal. The key results were that the fractal dimension of such clusters is four independent of the dimension of the imbedding space and different from the Hausdorf dimension and that the density of these clusters is significantly less than the value predicted by the scaling of the order parameter as would be expected in systems that have hyperscaling.

Publications 1 and 2

2. Clusters in nucleation near the spinodal singularity in liquid-gas like transitions

The structure of critical or nucleation droplets was studied in the proximity of the classical spinodal in Ising models. It was shown that the critical droplets could be described as clusters the structure of which could be determined by mapping the thermal spinodal singularity onto a percolation model. The linear size of these droplets or clusters was seen to be proportional to the thermal correlation length which diverges as the spinodal is approached. Moreover the density difference between the interior of the droplet or cluster was seen to vanish as the spinodal is approached.

Publications 2 and 3

3. Clusters in nucleation near the spinodal in crystallization

The nucleation process in crystallization is very poorly understood. It is known that there are spinodals in supercooled liquids in systems with long range interactions but the effect of such spinodals on the nucleation process has not been elucidated. We performed large scale molecular dynamics simulations to investigate this phenomenon. Unfortunately the precise definition of clusters available for the work on spinodal nucleation in Ising models is not as yet available for fluids so we developed phenomenological cluster definitions. Two major conclusions emerged from this work.

a. There appeared to be non classical nucleation phenonena in deeply quenched Lennard-Jones, r^{-6} and r^{-12} potentials which was consistent with a spinodal nucleation interpretation.

b. More theoretical and numerical investigations are necessary to determine the cause of the observed non classical effects.

To this end we have developed molecular dynamics code for the Connection Machine. Code for the CM-2 has been written and code for the CM-5 is being developed.

In addition we have begun to develop a language to treat continuum percolation with the goal to find a precise cluster description of droplets near the spinodal in super-cooled liquids.

Publications 4, 5, 6, 7 and 8

4. Clusters in spinodal decomposition and continuous ordering

The phenomena of continuous ordering and spinodal decomposition are not well understood. The so-called linear theory or Cahn-Hilliard-Cook theory has a temporal range of validity that increases with interaction range but a description of the crossover to the non-linear regime as well as a reasonable theory for the early non-linear evolution is not available. In order to facilitate the development of such a theory we have begun to investigate the linear regime and its breakdown.

To that end we have mapped the linear regime of spinodal decomposition and continuous ordering onto a cluster growth problem, analyzed the fractal and mutifractal structures that appear and have begun to investigate the crossover to the non-linear behavior.

We have also begun an extensive numerical investigation of the early stages of spinodal decomposition and continuous ordering.

Publications 9 and 10

5. Cluster acceleration algorithms

One of the major impediments to obtaining better numerical data on the kinetics of phase transitions is the time required to complete a run from the initial equilibrium state, through the quench into the metastable or unstable state and finally to the new equilibrium state. The time constraints lead to simulations of small systems with the attendent finite size effects. In order to speed up the simulations we have begun to investigate the possible application of the new cluster acceleration algorithms introduced to study equilibrium critical phenomena to problems in the kinetics of phase transitions.

We have proposed an explanation of why the algorithms work as well as examining their dimensional dependence. We have also begun to investigate the generalization of these algorithms, constructed for systems with no conserved quantities, to models with a conserved order parameter.

Publications 11, 12, 13 and 14

Publications 1 October 1987 - 30 September 1990

1. T. Ray and W. Klein, J. Stat. Phys. **53**, 773 (1988)
2. T. Ray and W. Klein, J. Stat. Phys. **61**, 891 (1990)
3. L. Monette, W. Klein, M. Zuckermann, A. Khadir and R. Harris, Phys. Rev. **B38**, 11874 (1988)
4. J. Yang, H. Gould and W. Klein, Phys. Rev. Lett. **60**, 2655 (1988)
5. J. Yang, H. Gould, W. Klein and R. Mountain, J. Chem. Phys. **93**, 711 (1990)
6. A. Melcuk, R. Giles and H. Gould, Computers in Physics 5, 331 (1991)
7. J. Given and W. Klein, Phys. Rev. **B38**, 11874 (1988)
8. J. Given and W. Klein, J. Chem Phys. **90**, 1116 (1989)
9. M. Laradji, M. Grant, M. Zuckermann and W. Klein, Phys. Rev. **B41**, 4646 (1990)
10. W. Klein, Phys. Rev. Lett. **65**, 1462 (1990)
11. W. Klein, T. Ray and P. Tamayo, Phys. Rev. Lett. **62**, 163 (1989)
12. T. Ray, P. Tamayo and W. Klein, Phys. Rev. **A39**, 5949 (1989)
13. P. Tamayo and W. Klein, Phys. Rev. Lett. **63**, 2757 (1989)
14. P. Tamayo, R. Brower and W. Klein, J. Stat. Phys. **58**, 1083 (1990)

Statement A per telecon Dr. Peter Reynolds
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Students Supported by This Grant

1. J. Given, PhD 1988 - Currently a Post Doctoral Fellow wit G. Stell at SUNY Stony Brook

2. T. S. Ray, PhD 1989 - Currently a Post Doctoral Fellow wit C. Döring at Clarkson University

3. L. Monette, PhD 1990 - Currently a Post Doctoral Fellow with Gary Grest and Micheal Andersen at Exxon Research

4. P. Tamayo, PhD 1990 - Currently a Post Doctoral Fellow at Thinking Machines Corporation

5. J. S. Yang, PhD 1990 - Currently a Post Doctoral Fellow at CUNY with Joel Koplick

Presentations of Supported Work

W. Klein

1. Seminar-National Bureau of Standards, Feb. 1988
2. Seminar-IBM, Yorktown Heights, May 1988
3. Seminar-IBM, Bergen Norway, July 1988
4. Invited Speaker-Workshop on "Simulations in Physics" Trieste, Italy July 1988
5. Seminar-Nordita, Copenhagen, Dennmark, August 1988
6. Seminar-Technical University of Dennmark, August 1988
7. Invited Speaker-American Metallurgical Society, Sept. 1988
8. Seminar-Brown University, Nov. 1988
9. Invited Speaker-USGS Meeting, Stat. Mech. and Earthquakes, Asilomar CA, Feb. 1989
10. Seminar-Stanford University, Feb. 1989
11. Seminar-Sandia Laboratory, Nov. 1989
12. Invited Speaker-MRS Meeting, Boston MA, Nov. 1989
13. Seminar-IBM Almaden, CA Jan. 1990
14. Seminar-Lawrence Livermore Laboratory, Jan. 1990
15. Invited Speaker-Workshop, Comp. Simulation in Phys., Univ. of Georgia, Feb. 1990
16. Seminar-Emory University, Feb. 1990
17. Seminar-McGill University, Feb. 1990
18. Seminar-Florida State University, May 1990
19. Invited Speaker-SIAM Meeting, Orlando FL, May 1990
20. Seminar-Carnegie-Mellon University, July 1990
21. Seminar-UCLA, August 1990
22. Titan Corporation, San Diego, CA, August 1990